Reconstructing Polyatomic Structures from Discrete X-Rays: NP-Completeness Proof for Three Atoms

Marek Chrobak* Christoph Dürr[†]

Abstract

We address a discrete tomography problem that arises in the study of the atomic structure of crystal lattices. A polyatomic structure T can be defined as an integer lattice in dimension $D \geq 2$, whose points may be occupied by c distinct types of atoms. To "analyze" T, we conduct ℓ measurements that we call discrete X-rays. A discrete X-ray in direction ξ determines the number of atoms of each type on each line parallel to ξ . Given ℓ such non-parallel X-rays, we wish to reconstruct T.

The complexity of the problem for c=1 (one atom type) has been completely determined by Gardner, Gritzmann and Prangerberg [5], who proved that the problem is NP-complete for any dimension $D \geq 2$ and $\ell \geq 3$ non-parallel X-rays, and that it can be solved in polynomial time otherwise [9].

The NP-completeness result above clearly extends to any $c \ge 2$, and therefore when studying the polyatomic case we can assume that $\ell = 2$. As shown in another article by the same authors, [4], this problem is also NP-complete for $c \ge 6$ atoms, even for dimension D = 2 and axis-parallel X-rays. The authors of [4] conjecture that the problem remains NP-complete for c = 3, 4, 5, although, as they point out, the proof idea in [4] does not seem to extend to $c \le 5$.

We resolve the conjecture from [4] by proving that the problem is indeed NP-complete for $c \geq 3$ in 2D, even for axis-parallel X-rays. Our construction relies heavily on some structure results for the realizations of 0-1 matrices with given row and column sums.

^{*}Department of Computer Science, University of California, Riverside, CA 92521-0304. Email marek@cs.ucr.edu. Research supported by NSF grant CCR-9503498. This research was partially conducted when the author was visiting International Computer Science Institute in Berkeley.

[†]International Computer Science Institute, 1947 Center Street, Suite 600, Berkeley, CA 94704-1198. Email cduerr@icsi.berkeley.edu. URL http://www.icsi.berkeley.edu/~cduerr/%Xray.

1 Introduction

The fundamental principle of the transmission electron microscope (TEM) is very similar to the more familiar optical microscope: it "shines" a focused beam of electrons towards a specimen, and the transmitted beam is projected onto a phosphor screen, thereby generating an image. The intensity represents the density and thickness of the specimen: denser or thicker areas of the specimen transmit fewer electrons and produce darker areas in the image. The development of the TEM in 1930's was necessitated by the limitations of the optical microscopes, whose magnification and resolution were insufficient to study the internal structure of organic cells or to find defects in bulk materials. Recently, new advancements in high-resolution TEM (HRTEM) led to the development of instruments and techniques for studying biological molecules and for investigating the atomic structure of crystals. In particular, a technique called QUANTITEM [8, 10] allows one to determine the number of atoms in the atom columns of a crystal in certain directions. Given these numbers, we wish to reconstruct the structure of the crystal. This is an example of an algorithmic problem belonging to discrete tomography, the area of mathematics and computer science that deals with inverse problems of reconstructing discrete density functions from a finite set of projections. The size of crystals that occur in materials science applications is about 10^6 atoms, and, for data sets that large, efficient reconstruction algorithms would be of great interest.

The problem we address in this paper can be formulated as follows: Define a polyatomic structure T as an integer lattice in dimension $D \geq 2$, whose cells may be occupied by c distinct types of atoms. Each of these cells can be occupied by one atom, or it could be empty. To "analyze" T, we conduct ℓ measurements that we refer to as discrete X-rays. (QANTITEM uses electron beams, but, following [5], we use a more familiar term "X-ray" instead.) A discrete X-ray in direction ξ determines the number of atoms of each type on each line parallel to ξ . Given such ℓ non-parallel X-rays, we wish to reconstruct T.

The complexity of the problem for c=1 (one atom type) has been completely determined by Gardner, Gritzmann and Prangerberg [5], who proved that the problem is NP-hard for any dimension $D \geq 2$ and $\ell \geq 3$ non-parallel X-rays, and that it can be solved in polynomial time otherwise [9].

The NP-hardness result above clearly extends to any $c \geq 2$, and therefore when studying the polyatomic case we can assume that $\ell = 2$. As shown in another article by the same authors, [4], this problem is also NP-hard for $c \geq 6$ atoms, even for dimension D = 2 and for the axis-parallel X-rays. The authors of [4] conjectured that the problem remains NP-hard for c = 3, 4, 5, and they pointed out that for these values of c "a substantially new technique will be needed, at least for the case c = 3".

We resolve the conjecture from [4] by proving that the problem is indeed NP-hard for c=3 (and thus for any larger c as well) in 2D, even for the orthogonal case, that is, with axis-parallel X-rays.

In the orthogonal case, the problem is equivalent to that of reconstructing (c+1)-valued matrices (c atom types and "holes") from the row and column sums for each atom. Without loss of generality, we can concentrate on square, say $L \times L$, matrices. Let Δ be the set of c atom types. For any atom type $a \in \Delta$, denote by r_i^a (resp. s_j^a) the row-sum (resp. column-sum) of atom a, that is, the number of atoms of type a in row i (resp. in column j). The vectors $\mathbf{r}^a = (r_1^a, \ldots, r_L^a)$ and $\mathbf{s}^a = (s_1^a, \ldots, s_L^a)$ are referred to, respectively, as the row-sum vector and the column-sum vector for atom a.

A realization of the sums $\mathcal{I} = (\mathbf{r}^a, \mathbf{s}^a)_{a \in \Delta}$ is an $L \times L$ matrix T with values from $\Delta \cup \{\Box\}$, such

that for each atom type $a \in \Delta$

$$egin{array}{lll} |\{j:T[i,j]=a\}| &=& r_i^a & \forall i=1,\ldots,L \ |\{i:T[i,j]=a\}| &=& s_j^a & \forall j=1,\ldots,L \end{array}$$

We say that \mathcal{I} is *consistent* if it has a realization.

More specifically, we concentrate on the following decision problem:

c-Color Consistency Problem (c-CCP)

Instance: row and column sums $\mathcal{I} = (\mathbf{r}^a, \mathbf{s}^a)_{a \in \Delta}$, where $|\Delta| = c$;

Query: Is \mathcal{I} consistent?

Gardner, Gritzmann and Prangerberg proved in [4] that 6-CCP is NP-complete. In this paper we prove that 3-CCP is NP-complete.

If we restrict ourselves further to just one atom (that is, 1-CCP), the problem becomes equivalent to the reconstruction of 0-1 matrices from the row and column sums – a problem predating the discrete tomography research. The first efficient reconstruction algorithm was proposed in 1963 by Ryser [9], and a similar algorithm was rediscovered in 1971 by Chang [2]. In addition to reconstruction, Ryser and others studied various structural properties of 0-1 matrices with given row and column sums, and our construction relies heavily on some results in this area. Interested readers are referred to an excellent survey by Brualdi [1].

The general idea of the proof is explained in Section 2. In Section 3, we review the structural properties of 0-1 matrices with given row and column sums that are needed for our proof. Using these properties, we prove the Skew-Mirror Lemma in Section 4. In Section 5, we construct a number of gadgets, including "skew mirrors" and "edge verifiers", and we prove that they satisfy the desired properties. Finally, in Section 6, we present the complete construction and give the formal NP-completeness proof.

In addition to the QUANTITEM method, the problem of reconstructing lattice sets from their projections arises naturally in a variety of other areas, including statistics, data security, and image processing. It can also be expressed as a multicommodity flow problem. We discuss these issues in Section 7, where we also comment on the last unresolved case, c = 2.

2 The General Idea of the Proof

In the proof, we use a reduction from the Vertex Cover problem:

Vertex Cover Problem

Instance: An undirected graph G(V, E), an integer K;

Query: Is there a vertex cover of G of size K?

Recall that a vertex cover of a graph G = (V, E) is a set $U \subseteq V$ such that for all $(u, v) \in E$, either $u \in U$ or $v \in U$. The Vertex Cover problem is well known to be NP-complete (see, for example, [6]). Let n = |V| and m = |E|. We assume, without loss of generality, that $m, n \ge 1$.

Suppose first that using some set Δ' of d atom types, we can force a unique realization of the form shown in Figure 1. We call this realization a *frame*. In the frame, the empty entries form two diagonals, the *main diagonal* of length (m+1)n, and the *side diagonal* of length mn. We divide

both diagonals into intervals of length n that we refer to as mirrors. Thus we have two rows of mirrors: m+1 mirrors in the main-diagonal, and m mirrors in the side-diagonal. All other entries are filled with atoms from Δ' .

We now add two more atom types $C, D \notin \Delta'$. Use atom D to create m copies of a candidate vertex cover U in the following way: The first row and column D-sum is K and all other D-sums are 1. (Figure 1 shows the D-sums.) Then the pattern of Ds in each main-diagonal mirror is the same, and is also the same as the pattern of holes in the side-diagonal mirrors. We associate U with this pattern: a vertex u is in U iff the uth cell in any side-diagonal mirror is a hole. We think of U as a "beam" projected onto the last n cells in the first column, repeatedly reflected in a double-row of mirrors, and exiting through the last n cells in the first row.

Finally, we can use atom C to verify that U is indeed a vertex cover. In order to do so, we convert the jth side-diagonal mirror into an edge verifier for edge e_j

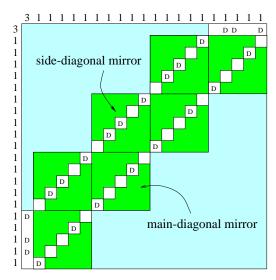


Figure 1: The frame and mirrors for m = 3.

(u, v) (it may be necessary to add some more rows and columns to the matrix shown in Figure 1). Using appropriate sums for atom C, the realization of atoms in Δ' can be extended to a realization of all atoms, including C, iff either the uth cell or the vth cell in side-diagonal mirrors is a hole (and thus, either $u \in U$ or $v \in U$).

An idea similar to the one described above was used by Gardner, Gritzmann and Prangerberg [4] (they used a reduction from a different problem, not Vertex Cover). Using 4 atoms they constructed, in essence, what we call a frame, obtaining the NP-completeness proof for 6 atoms. We were able to construct the frame gadget with only 3 atoms, reducing the total number of atoms to 5. However, this idea does not work when fewer than 5 atoms are available. As pointed out by [4], a new approach is needed.

The main idea behind our proof is this: Define a partial order " \preceq " on all K-element vertex sets (candidate vertex covers). The important property of " \preceq " is that its depth is polynomial, namely at most J = K(n-K) + 1 (each strictly increasing chain has length at most J). Further, " \preceq " has a unique minimum element U^{min} , and a unique maximum element U^{max} . Instead of using "perfect" mirrors, we use "skew" mirrors. These mirrors have the property that the reflected set is never smaller (with respect to partial order " \preceq ") than the set projected onto a skew mirror. These skew mirrors are also "wobbly" — we know that they can reflect the same or a bigger set, but we cannot control what exactly the reflected set will be.

Now, instead of using m mirrors, we use mJ skew mirrors in the side-diagonal. They are divided into J segments of m mirrors each. In each segment, the jth skew mirror is converted into an edge verifier for edge e_j . We "shine" U^{min} onto the first mirror in the bottom-left corner, and we make sure that the final set resulting from all reflections in the top-right corner is U^{max} . Since " \preceq " has depth J, there has to be a segment in which all mirrors reflect the same set U. Then the edge verifiers in this segment will verify that U is indeed a vertex cover.

Why does it help? It turns out that our skew mirrors can be constructed using only two atom types. Furthermore, the same atom types can be used to encode the information about the

candidate vertex cover U. We use one more atom type to construct edge verifiers, and thus we only need three atom types for the whole construction.

3 0-1 Matrices with Given Row and Column Sums

In this section we review some basic results from the literature on 0-1 matrices with given row and column sums.

By $\mathbf{x}, \mathbf{y}, \mathbf{z}$ we denote nonnegative integer vectors of length p, for example $\mathbf{x} = (x_1, \dots, x_p)$. The reconstruction problem for 0-1 matrices with given row and column sums is equivalent to 1-CCP, and can be stated as follows: Given \mathbf{x} and \mathbf{y} , is there a 0-1 matrix T that has x_i 1's in row i and y_j 1's in column j, for all $1 \leq i, j \leq p$? Again, in this case, a matrix T satisfying these conditions is called a realization, and \mathbf{x}, \mathbf{y} are called consistent if they have a realization.

The structure function. Given a $p \times p$ matrix T, and integers $0 \le k, l \le p$ we partition T into four submatrices (which may have zero width or height): T_{kl}^{\square} , T_{kl}^{\square} , T_{kl}^{\square} and T_{kl}^{\square} defined by the intersections of the first k rows (resp. last p-k rows) and the first l columns (resp. last p-l columns), that is

$$T = \left(egin{array}{cc} T_{kl}^{lacksquare} & T_{kl}^{lacksquare} \ T_{kl}^{lacksquare} & T_{kl}^{lacksquare} \end{array}
ight).$$

By $|T|_1$ and $|T|_0$ we denote the numbers of 1's and 0's in matrix T. For a given instance \mathbf{x}, \mathbf{y} , the *structure function* τ_{kl} is defined by

$$\tau_{kl} = (p-k)(p-l) + \sum_{j=1}^{l} y_j - \sum_{i=k+1}^{p} x_i.$$

Then for any arbitrary realization T we have

$$\tau_{kl} = (p-k)(p-l) + \sum_{j=1}^{l} y_j - \sum_{i=k+1}^{p} x_i
= |T_{kl}|_0 + |T_{kl}|_1 + |T_{kl}|_1 + |T_{kl}|_1 - |T_{kl}|_1 - |T_{kl}|_1
= |T_{kl}|_0 + |T_{kl}|_1$$
(1)

Consistent sums. We now show that, using the structure function, it is possible to characterize consistent sums. An integer vector $\mathbf{z} = (z_1, \dots, z_p)$ will be called *monotone* if $z_1 \leq \dots \leq z_p$.

Lemma 1 [1] Monotone vectors \mathbf{x}, \mathbf{y} are consistent if and only if $\tau_{kl} \geq 0$ for all $k, l = 1, \ldots, p$.

The implication (\Rightarrow) in Lemma 1 follows directly from Equation (1). The implication (\Leftarrow) can be proven constructively by giving an algorithm that produces a realization T for any pair (\mathbf{x}, \mathbf{y}) for which the structure function is non-negative. (See [1] for details.) It is also not hard to see that Lemma 1 can be derived from the Max-Flow-Min-Cut theorem for network flows.

Decomposed realizations. We say that T is (k,l)-decomposed if T_{kl}^{\square} consists only of 0's and T_{kl}^{\square} consists only of 1's. The lemma below follows immediately from Equation (1), and it will play a major role in this paper.

Lemma 2 [1] Suppose that T is a realization of (\mathbf{x}, \mathbf{y}) , and let $0 \le k, l \le p$. Then $\tau_{kl} = 0$ if and only if T is (k, l)-decomposed.

Remark 1 Lemma 2 implies that if just one realization of \mathbf{x} , \mathbf{y} is (k, l)-decomposed, then all realizations are (k, l)-decomposed as well.

4 The Skew-Mirror Lemma

0-1 Vectors and minorization. We use Greek letters $\boldsymbol{\alpha}, \boldsymbol{\beta}, \ldots$ for 0-1 vectors of length p, say $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_p)$. The complement $\bar{\boldsymbol{\alpha}}$ of $\boldsymbol{\alpha}$ is $\bar{\alpha}_i = 1 - \alpha_i$ for all $i = 1, \ldots, p$, and the reverse $\bar{\boldsymbol{\alpha}}$ is $\bar{\alpha}_i = \alpha_{p-i+1}$ for $i = 1, \ldots, p$.

We say that α minorizes β , denoted $\alpha \prec \beta$, if

$$\sum_{i=1}^{k} \alpha_i \leq \sum_{i=1}^{k} \beta_i \quad \forall k = 1, \dots, p.$$

By straightforward verification, " \leq " is a partial order. We also write $\alpha \prec \beta$ if $\alpha \leq \beta$ and $\alpha \neq \beta$. The *total sum* of a 0-1 vector α is $\Sigma \alpha = \sum_{i=1}^{p} \alpha_i$. If α , β are two 0-1 vectors with equal total sums, then the definitions above imply directly the following equivalences:

$$\alpha \preceq \beta \iff \bar{\alpha} \succeq \bar{\beta} \iff \bar{\alpha} \succeq \bar{\beta}.$$

An important property of the minorization relation is that it is "shallow", that is its depth is only polynomial (unlike, for example, the lexicographic order). The next lemma gives a more accurate estimate on the depth of "\(\triangleq \)".

Lemma 3 Suppose that we have a strictly increasing sequence of 0-1 vectors

$$\alpha^1 \prec \alpha^2 \prec \ldots \prec \alpha^q$$

with total sums $\Sigma \alpha^i = t$ for each i. Then $q \leq t(p-t) + 1$.

Proof To each 0-1 vector $\boldsymbol{\alpha}$ assign the number $\|\boldsymbol{\alpha}\|$ defined by

$$\|\boldsymbol{\alpha}\| = \sum_{j=1}^{p} (p-j+1)\alpha_j = \sum_{k=1}^{p} \sum_{i=1}^{k} \alpha_i.$$

If $\alpha \prec \beta$ then $\sum_{i=1}^k \alpha_i \leq \sum_{i=1}^k \beta_i$ for k = 1, ..., p, and this inequality must be strict for at least one k. We conclude that $\alpha \prec \beta$ implies $\|\alpha\| < \|\beta\|$.

Now, by the argument above, the numbers $\|\alpha^i\|$ are strictly increasing. Therefore

$$q \le \|\alpha^q\| - \|\alpha^1\| + 1$$
 $\le \sum_{k=p-t+1}^p k - \sum_{k=1}^t k + 1$
 $= t(p-t) + 1,$

completing the proof.

The 0-1 skew mirror. The lemma below deals with a special instance of the reconstruction problem for 0-1 matrices, in which the row sum vector \mathbf{x} is determined by a 0-1 vector $\boldsymbol{\alpha}$, and the column-sum vector \mathbf{y} is determined by a 0-1 vector $\boldsymbol{\beta}$.

Given a 0-1 vector $\boldsymbol{\sigma}$ of length p, we associate with $\boldsymbol{\sigma}$ a $p \times p$ perfect mirror matrix $PM_{\boldsymbol{\sigma}}$ defined by

$$PM_{\sigma}[i,j] = \begin{cases} 0 & \text{for } i+j \leq p \\ \sigma_i & \text{for } i+j = p+1 \\ 1 & \text{for } i+j \geq p+2 \end{cases}$$

In a perfect-mirror matrix the cells on the main diagonal i + j = p + 1, counted from top down, contain σ , while all cells above it are 0, and all cells below it are 1 (see Figure 2b). From Lemma 2 we immediately obtain the following corollary.

Corollary 1 Let σ be a 0-1 vector of length p. Then PM_{σ} is a realization of vectors \mathbf{x}, \mathbf{y} if and only if for each $k = 1, \ldots, p$, (a) $\tau_{k,p-k} = 0$, and (b) $\tau_{k,p+1-k} = 0$ iff $\sigma_k = 0$.

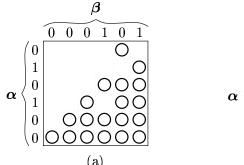
Note that Corollary 1 implies that if PM_{σ} is a realization of \mathbf{x}, \mathbf{y} then it is unique.

Lemma 4 Let α , β be two 0-1 vectors of length p, and let \mathbf{x} , \mathbf{y} be row and column sums defined by $x_i = i - \alpha_i$ and $y_i = i - \beta_i$, for $i = 1, \ldots, p$. Then

- (a) Vectors \mathbf{x}, \mathbf{y} are consistent iff $\Sigma \mathbf{\bar{\alpha}} = \Sigma \boldsymbol{\beta}$ and $\mathbf{\bar{\alpha}} \succeq \boldsymbol{\beta}$.
- (b) Suppose that \mathbf{x}, \mathbf{y} are consistent. Then $\overleftarrow{\boldsymbol{\alpha}} = \boldsymbol{\beta}$ iff the unique realization of \mathbf{x}, \mathbf{y} is $PM_{\overleftarrow{\boldsymbol{\alpha}}}$.

Proof Vectors \mathbf{x} , \mathbf{y} are monotone, so we can use Lemma 1. We start by computing the structure function for \mathbf{x} and \mathbf{y} :

$$\tau_{kl} = (p-k)(p-l) + \sum_{j=1}^{l} y_j - \sum_{i=k+1}^{p} x_i
= (p-k)(p-l) + \sum_{j=1}^{l} (j-\beta_j) - \sum_{i=k+1}^{p} (i-\alpha_i)
= \sum_{i=k+1}^{p} \alpha_i - \sum_{j=1}^{l} \beta_j + \frac{1}{2} [2(p-k)(p-l) - p(p+1) + k(k+1) + l(l+1)]
= \sum_{i=1}^{p-k} \overline{\alpha}_i - \sum_{j=1}^{l} \beta_j + \frac{1}{2} (p-k-l-1)(p-k-l)$$
(2)



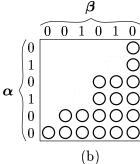


Figure 2: (a) A realization of x, y for $\alpha = 010100$ and $\beta = 000101$. We write 0-1 vectors as binary strings, for simplicity. Disks represent 1's. (b) Perfect mirror PM_{σ} for $\sigma = 101011$.

Now we are ready to prove Part (a). We prove the two implications separately.

- (\Rightarrow) For any $l=0,\ldots,p$, using Equation (2) with k=p-l, we get that $\tau_{p-l,l}\geq 0$ implies $\sum_{i=1}^{l} \overline{\alpha}_i \sum_{j=1}^{l} \beta_j \geq 0$. Thus $\overline{\boldsymbol{\alpha}} \succeq \boldsymbol{\beta}$. Moreover, \mathbf{x} and \mathbf{y} have equal total sums, if and only if $\Sigma \boldsymbol{\alpha} = \Sigma \boldsymbol{\beta}$.
- (\Leftarrow) Assume that $\overleftarrow{\alpha} \succeq \beta$. We consider two cases, when $k+l \leq p$ and $k+l \geq p+1$. Suppose first that $k+l \leq p$. From Equation (2) we have

$$\tau_{kl} = \sum_{i=1}^{l} \overleftarrow{\alpha}_i + \sum_{i=l+1}^{p-k} \overleftarrow{\alpha}_i - \sum_{j=1}^{l} \beta_j + \frac{1}{2} (p-k-l-1)(p-k-l) \\
\geq 0,$$

because $\sum_{i=1}^{l} \overline{\alpha}_i - \sum_{j=1}^{l} \beta_j \ge 0$, and $(p-k-l-1)(p-k-l) \ge 0$.

Suppose now that $k + l \ge p + 1$. From Equation (2) we have

$$\tau_{kl} = \sum_{i=1}^{l} \overleftarrow{\alpha}_{i} - \sum_{i=p-k+1}^{l} \overleftarrow{\alpha}_{i} - \sum_{j=1}^{l} \beta_{j} + \frac{1}{2} (p-k-l-1)(p-k-l)$$

$$= \sum_{i=1}^{l} \overleftarrow{\alpha}_{i} - \sum_{j=1}^{l} \beta_{j} - \sum_{i=p-k+1}^{l} \overleftarrow{\alpha}_{i} + \frac{1}{2} (k+l+1-p)(k+l-p)$$

$$= \sum_{i=1}^{l} \overleftarrow{\alpha}_{i} - \sum_{j=1}^{l} \beta_{j} + \frac{1}{2} \sum_{i=p-k+1}^{l} (k+l+1-p-2\overleftarrow{\alpha}_{i})$$

$$> 0.$$

because $\sum_{i=1}^{l} \overline{\alpha}_i - \sum_{j=1}^{l} \beta_j \geq 0$, and $k+l+1-p-2\overline{\alpha}_i \geq 2-2\overline{\alpha}_i \geq 0$.

Now we prove Part (b). By Corollary 1 and Equation (2), a realization of \mathbf{x}, \mathbf{y} is a perfect mirror $PM_{\boldsymbol{\sigma}}$, for some $\boldsymbol{\sigma}$, if and only if $\boldsymbol{\bar{\alpha}} = \boldsymbol{\beta}$. Thus it is sufficient to show that $\boldsymbol{\bar{\alpha}} = \boldsymbol{\beta}$ implies that $\boldsymbol{\sigma} = \bar{\boldsymbol{\alpha}}$. This follows by simple verification of row sums.

5 Some Useful Gadgets

In this section we begin to describe our construction. Recall that G, K is the given instance of Vertex Cover, where G = (V, E), n = |V| and m = |E|. Without loss of generality we can assume that $0 \le K \le n$.

Throughout the rest of the paper we will use capital letters A, B, C to denote the three atom types, and we will sometimes refer to these types as colors: \underline{Azure} , \underline{Beige} , and \underline{Cyan} .

Beige skew mirror. Given two 0-1 vectors $\boldsymbol{\alpha}, \boldsymbol{\beta}$ of length n, we define the *beige skew mirror* as a $(n+2) \times (n+2)$ instance of 3-CCP, $BSM(\boldsymbol{\alpha}, \boldsymbol{\beta}) = (\mathbf{x}^B, \mathbf{y}^B)$, with the following row and column sums:

$$x_i^B = i - \alpha_i + 2$$
 $y_i^B = i - \beta_i + 2$ for $i = 1, ..., n$
 $x_i^B = n + 2$ $y_i^B = n + 2$ for $i = n + 1, n + 2$

The azure and cyan sums are zero.

Lemma 5 Let α, β be two 0-1 vectors of length n. Then $BSM(\alpha, \beta)$ is consistent if and only if $\Sigma \alpha = \Sigma \beta$ and $\overline{\alpha} \succeq \beta$.

Proof By definition, any realization of $BSM(\alpha, \beta)$ has its last 2 rows and last 2 columns completely filled with beige atoms. Define

$$x_i = x_i^B - 2 = i - \alpha_i,$$

 $y_i = y_i^B - 2 = i - \beta_i,$

where i = 1, ..., n. Then $BSM(\boldsymbol{\alpha}, \boldsymbol{\beta})$ is consistent if and only if the instance (\mathbf{x}, \mathbf{y}) of 1-CCP is consistent. Applying Lemma 4, we obtain that $BSM(\boldsymbol{\alpha}, \boldsymbol{\beta})$ is consistent if and only if $\Sigma \boldsymbol{\alpha} = \Sigma \boldsymbol{\beta}$ and $\boldsymbol{\alpha} \succeq \boldsymbol{\beta}$.

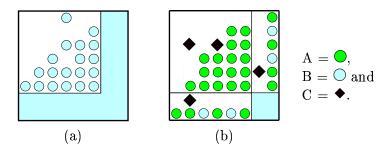


Figure 3: (a) A realization of BSM(010100,000011). (b) A realization of EV(010100,001010,(3,5)). Solid filled regions represent entries that are filled with beige atoms independently of the parameters of BSM and EV.

Azure skew mirror. Given two 0-1 vectors γ , δ of length n, we define the *azure mirror* as a $(n+2) \times (n+2)$ instance of 3-CCP, $ASM(\gamma, \delta) = (\mathbf{x}^A, \mathbf{y}^A, \mathbf{x}^B, \mathbf{y}^B)$, with the following row and

column sums:

The cyan sums are zero.

Lemma 6 Let γ, δ be two 0-1 vectors of length n such that $\Sigma \gamma = \Sigma \delta = n - K$. Then $ASM(\gamma, \delta)$ is consistent if and only if $\gamma \succeq \delta$.

Proof We claim that each realization of $ASM(\gamma, \delta)$ has being atoms on positions:

$$\begin{array}{ll} \{(i,n+2): \gamma_i = 1\} & \text{(last column)} \\ \{(n+2,i): \delta_i = 1\} & \text{(last row)} \\ \{(n+1,n+1), (n+1,n+2), (n+2,n+1), (n+2,n+2)\} & \text{(lower right } 2 \times 2 \text{ corner)} \end{array}$$

Since $x_{n+2}^B = n - K + 2$, and there are exactly n - K + 2 non-zero beige column sums, the beige atoms are determined uniquely, as shown above. Similarly, the beige atoms in the last column are determined uniquely. The last yet unallocated beige atom must be at (n + 1, n + 1).

We now examine azure atoms. Row n+1 and column n+1 have no azure atoms. In row n+2 azure atoms are forced to be in columns i for which $\delta_i = 0$, since all other positions are occupied by beige atoms. Similarly, in column n+2 azure atoms are in rows i for which $\gamma_i = 0$.

Let \mathbf{x}, \mathbf{y} be the following row and column sum vectors:

$$x_i = i - \bar{\gamma}_i y_i = i - \bar{\delta}_i,$$

for $i=1,\ldots,n$. Then $ASM(\boldsymbol{\gamma},\boldsymbol{\delta})$ is consistent iff the instance (\mathbf{x},\mathbf{y}) of 1-CCP is consistent. By Lemma 4, this is equivalent to $\boldsymbol{\bar{\gamma}}\succeq \boldsymbol{\bar{\delta}}$, or $\boldsymbol{\gamma}\succeq \boldsymbol{\bar{\delta}}$, completing the proof.

Edge verifier. For two 0-1 vectors γ , δ of length n, and for an edge e = (u, v) (with u < v) we define the *edge verifier* for e, as a $(n + 2) \times (n + 2)$ instance of 3-CCP,

$$EV(\boldsymbol{\gamma}, \boldsymbol{\delta}, e) = (\mathbf{x}^{A}, \mathbf{y}^{A}, \mathbf{x}^{B}, \mathbf{y}^{B}, \mathbf{x}^{C}, \mathbf{y}^{C}),$$

where the azure and beige sums are exactly the same as in the azure skew mirror $ASM(\gamma, \delta)$, and the cyan sums are:

Lemma 7 Let γ be a 0-1 vector of length n, and e = (u, v) (with u < v) be an edge of G. Then $EV(\gamma, \dot{\gamma}, e)$ is consistent if and only if $\Sigma \gamma = n - K$ and either $\gamma_u = 0$ or $\gamma_v = 0$.

Lemma 7 has the following interpretation: if we associate with γ the vertex set $U = \{u : \gamma_u = 0\}$, then $EV(\gamma, \overline{\gamma}, e)$ is consistent if and only if at least one endpoint of edge e belongs to U.

Proof We can assume that $\Sigma \gamma = n - K$. By Lemma 6, $ASM(\gamma, \overleftarrow{\gamma})$ is consistent. Furthermore, by Part (b) of Lemma 4, for any $1 \le i, j \le n$, a realization T of $ASM(\gamma, \overleftarrow{\gamma})$, satisfies: $T[i,j] = \square$ for $i+j \le n$, T[i,j] = A, for $i+j \ge n+2$, and for i+j = n+1 we have the following equivalence: $T[i,j] = \square$ iff $\gamma_i = 0$.

If $EV(\gamma, \overline{\gamma}, e)$ is consistent, we can extend T to a realization of $EV(\gamma, \overline{\gamma}, e)$, and consider the positions of cyan atoms. The position (n+1, n+1) contains a beige atom and (v, n-u+1) an azure atom. This leaves these possible positions for the cyan atoms:

$$(u, n-v+1)$$
 $(u, n-u+1)$ $(u, n+1)$ $(v, n-v+1)$ $(v, n+1)$ $(v, n+1)$ $(n+1, n-v+1)$

We claim that either T[u, n-u+1]=C or T[v, n-v+1]=C. For otherwise, the cyan row sums $x_u^C=2$ and $x_v^C=1$ force T[u, n+1]=T[v, n+1]=C, contradicting $y_{n+1}^C=1$.

In summary, we get that $EV(\gamma, \overleftarrow{\gamma}, e)$ is consistent iff one of γ_u, γ_v equals 0.

6 The Proof of NP-Completeness

6.1 The reduction

Recall that G = (V, E), K is the given instance of Vertex Cover, where |V| = n, |E| = m and $0 \le K \le n$. Define J = K(n - K) + 1 and L = (mJ + 1)(n + 2). We now show how to map G, K into an $L \times L$ instance of 3-CCP

$$\mathcal{I} = (\mathbf{r}^{A}, \mathbf{s}^{A}, \mathbf{r}^{B}, \mathbf{s}^{B}, \mathbf{r}^{C}, \mathbf{s}^{C}).$$

To specify the sums in \mathcal{I} , it is convenient to view $L \times L$ -matrices as being partitioned into $(mJ+1)^2$ submatrices of size $(n+2) \times (n+2)$, called *blocks*. A row or column index is then defined by its *block index* $a=0,\ldots,mJ$ and *offset* $i=1,\ldots,n+2$. For $a \neq mJ$ the azure and being sums are:

$$r_{a(n+2)+i}^{A} = s_{a(n+2)+i}^{A} = (mJ - a - 1)(n+2) + \begin{cases} i & i = 1, \dots, n \\ 0 & i = n+1 \\ K & i = n+2 \end{cases}$$

$$r_{a(n+2)+i}^{B} = s_{a(n+2)+i}^{B} = a(n+2) + \begin{cases} i+2 & i = 1, \dots, n \\ n+4 & i = n+1 \\ 2n+4-K & i = n+2 \end{cases}$$

and for a = mJ the azure sums are zero and the beige sums are

$$r_{a(n+2)+i}^{_B} = s_{a(n+2)+i}^{_B} = a(n+2) + \left\{ egin{array}{ll} i+2 & i=1,\ldots,K \\ i+1 & i=K+1,\ldots,n \\ n+2 & i=n+1,n+2 \end{array}
ight.$$

Finally, we define the cyan sums. For j = 0, ..., J-1 and k = 0, ..., m-1 let a = jm + k and b = mJ - 1 - a. If $e_k = (u, v)$ (with u < v), then

$$egin{array}{lll} r_{a(n+2)+u}^{\it C} &=& 2 & & s_{b(n+2)+n-u+1}^{\it C} &=& 1 \ r_{a(n+2)+n+1}^{\it C} &=& 1 & & s_{b(n+2)+n-v+1}^{\it C} &=& 2 \ r_{a(n+2)+n+1}^{\it C} &=& 1 & & s_{b(n+2)+n+1}^{\it C} &=& 1 \end{array}$$

The row and column sums not defined above are assumed to be zero.

6.2 Realizations of azure and beige atoms

Let \mathcal{A} and \mathcal{B} be $(n+2) \times (n+2)$ matrices completely filled with azure and beige atoms, respectively. We will use notation $\mathcal{A}(\gamma, \delta)$ for realizations of $ASM(\gamma, \delta)$ and $\mathcal{B}(\alpha, \beta)$ for realizations of $BSM(\alpha, \beta)$. We define π by

$$\boldsymbol{\pi} = \underbrace{0 \dots 0}_{K} \underbrace{1 \dots 1}_{n-K}$$

For 0-1 vectors $\boldsymbol{\beta}^0$, $\boldsymbol{\alpha}^0$, ..., $\boldsymbol{\beta}^{mJ-1}$, $\boldsymbol{\alpha}^{mJ-1}$, each of total sum n-K, consider $L \times L$ azure-and-beige matrices of the following form:

$$\begin{bmatrix} \mathcal{A} & \mathcal{A} & \mathcal{A} & \cdots & \mathcal{A}(\boldsymbol{\alpha}^{mJ-1}, \boldsymbol{\beta}^{mJ-1}) & \mathcal{B}(\boldsymbol{\alpha}^{mJ-1}, \boldsymbol{\pi}) \\ \mathcal{A} & \mathcal{A} & \mathcal{A} & \mathcal{B}(\boldsymbol{\alpha}^{mJ-2}, \boldsymbol{\beta}^{mJ-1}) & \mathcal{B} \\ \mathcal{A} & \mathcal{A} & \mathcal{A} & \mathcal{B} & \mathcal{B} \\ \vdots & & & \vdots \\ \mathcal{A} & \mathcal{A} & \mathcal{A}(\boldsymbol{\alpha}^{2}, \boldsymbol{\beta}^{2}) & \mathcal{B} & \mathcal{B} \\ \mathcal{A} & \mathcal{A}(\boldsymbol{\alpha}^{1}, \boldsymbol{\beta}^{1}) & \mathcal{B}(\boldsymbol{\alpha}^{1}, \boldsymbol{\beta}^{2}) & \mathcal{B} & \mathcal{B} \\ \mathcal{A}(\boldsymbol{\alpha}^{0}, \boldsymbol{\beta}^{0}) & \mathcal{B}(\boldsymbol{\alpha}^{0}, \boldsymbol{\beta}^{1}) & \mathcal{B} & \mathcal{B} & \mathcal{B} \\ \mathcal{B}(\boldsymbol{\pi}, \boldsymbol{\beta}^{0}) & \mathcal{B} & \mathcal{B} & \cdots & \mathcal{B} & \mathcal{B} \end{bmatrix}$$

$$(3)$$

Lemma 8 Let \mathcal{I}^{AB} be the restriction of \mathcal{I} to the azure and beige sums only. Then a matrix T is a realization of \mathcal{I}^{AB} if and only if T has the form (3), where

$$\boldsymbol{\pi} \preceq \boldsymbol{\dot{\beta}}^0 \preceq \boldsymbol{\alpha}^0 \preceq \boldsymbol{\dot{\beta}}^1 \preceq \boldsymbol{\alpha}^1 \preceq \ldots \preceq \boldsymbol{\dot{\beta}}^{mJ-1} \preceq \boldsymbol{\alpha}^{mJ-1} \preceq \boldsymbol{\dot{\pi}}. \tag{4}$$

Proof Note that by Lemma 5 and 6, a matrix of the form (3) exists iff inequalities (4) are true. (\Leftarrow) Let T be a matrix of the form (3). By straightforward verification of the row and column sums we obtain that T is a realization of \mathcal{I}^{AB} . (Note that the entries of α^i, β^i , $i = 0, \ldots, mJ - 1$ appear in the beige sums with the plus sign in the azure skew mirrors, and with the minus sign in the beige skew mirrors.)

 (\Rightarrow) Let now T be a realization of \mathcal{I}^{AB} , and denote by F an arbitrary matrix of the form (3). Block (a,b) consist of entries in rows a(n+2)+i and columns b(n+2)+j for all $i,j=1,\ldots,n+2$. We

call it

```
an upper-left block if a+b < mJ,
the side-diagonal block b if a+b=mJ,
the main-diagonal block b if a+b=mJ+1,
and a lower-right block if a+b > mJ+1.
```

We claim that T has the structure depicted in Figure 4. Let \bar{T}^A be the 0-1 matrix representing

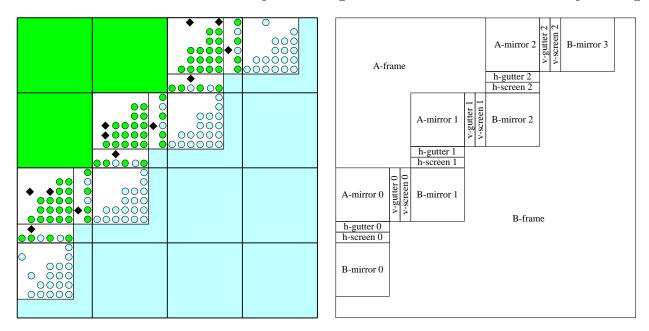


Figure 4: A realization of \mathcal{I} and its abstract structure. The pictures only illustrate the typical structure of a realization. (Since mJ is a large number for nontrivial graphs, it is not possible to draw an actual example of our construction.)

the non-azure cells in T: $\bar{T}^A[i,j]=1$ if and only if $T[i,j]\neq A$. Let \bar{F}^A be the analogous matrix for F. Then \bar{T}^A and \bar{F}^A are realizations of the same instance of 1-CCP. Therefore, if F^A is (k,l)-decomposed so must be T^A . Let k=(mJ-d)(n+2) and l=d(n+2) for any $d=0,\ldots,mJ$. Then \bar{F}^A is (k,l)-decomposed. Thus all upper-left blocks in T are exactly A and all main-diagonal and lower-right blocks have no azure atoms. The union of all upper-left blocks will be called the A-frame.

Let T^B be the 0-1 matrix T representing the beige atoms in T, that is $T^B[i,j]=1$ if and only if T[i,j]=B. Let F^B be the analogous matrix for F. Let k,l be a pair of indices such that either k=(mJ+1-d)(n+2)-2 and l=d(n+2)-2 for some $d=1,\ldots,mJ$, or $(k,l)\in\{(0,L-2),(L-2,0)\}$. Then, by the structure of realizations of azure and beige skew mirrors in Lemmas 5 and 6, F^B is (k,l)-decomposed, and so must be T^B . The region in T corresponding to the 1's in the submatrices T_{kl}^{\square} (for the k,l chosen above) is called the B-frame. So the B-frame of T is all beige. Since the lower-right blocks are included in this region, they are exactly B.

We partition the side-diagonal block b into

A-mirror b upper left $n \times n$ corner B-corner b lower right 2×2 corner v-screen b remaining entries in column n+2h-screen b remaining entries in row n+2

v-gutter b remaining entries in column n+1

h-gutter b remaining entries in row n+1.

Our previous observation implies that the B-corner is completely beige (as it is part of the B-frame), and the A-mirror does not contain any beige atoms. The gutters are completely empty and the screens completely filled, since

$$r_{b(n+2)+n+1}^{^{A}} + r_{b(n+2)+n+1}^{^{B}} = L - n = s_{b(n+2)+n+1}^{^{A}} + s_{b(n+2)+n+1}^{^{B}} + s_{b(n+2)+n+2}^{^{B}} = L = s_{b(n+2)+n+2}^{^{A}} + s_{b(n+2)+n+2}^{^{B}} + s_{b(n+2)+n+2}^{^{B}} + s_{b(n+2)+n+2}^{^{B}} + s_{b(n+2)+n+2}^{^{B}} = s_{b(n+2)+n+2}^{^{A}} + s_{b(n+2)+n+2}^{^{B}} + s_{b(n+2)+n+2}^$$

We define 0-1 vectors $\boldsymbol{\beta}^0, \boldsymbol{\alpha}^0, \dots, \boldsymbol{\beta}^{mJ-1}, \boldsymbol{\alpha}^{mJ-1}$ to represent positions of the beige atoms in the screens: $\alpha_i^b = 1$ if and only if *i*-th atom (from top) in v-screen *b* is beige and $\beta_i^b = 1$ if and only if *i*-th atom (from left) in h-screen *b* is beige.

Since the main-diagonal blocks have no azure atoms, each side-diagonal blocks b is a realization of $ASM(\boldsymbol{\alpha}^b, \boldsymbol{\beta}^b)$. Moreover, the main-diagonal blocks 0 and mJ are realizations of, respectively, $BSM(\boldsymbol{\pi}, \boldsymbol{\beta}^0)$ and $BSM(\boldsymbol{\alpha}^{mJ-1}, \boldsymbol{\pi})$, and each other main-diagonal block b, for $b=1,\ldots,mJ-1$, is a realizations of $BSM(\boldsymbol{\alpha}^{b-1}, \boldsymbol{\beta}^b)$. Lemmas 5 and 6 imply inequalities (4).

6.3 The Correctness Proof

Theorem 1 The problem 3-CCP is NP-complete in the strong sense.

Proof Clearly, 3-CCP is in NP. To justify the correctness of the reduction described in Section 6.1, we need to prove that G has a vertex cover of size K if and only if \mathcal{I} is consistent.

- (\Rightarrow) Suppose that U is a vertex cover of size K in G. Define γ by $\gamma_u = 0$ iff $u \in U$. Let T be a matrix of the form (3) in which $\alpha^i = \gamma$, and $\beta^i = \overleftarrow{\gamma}$ for $i = 0, \ldots, mJ 1$. We have $\pi \preceq \gamma \preceq \overleftarrow{\pi}$. By Lemma 8, T is a realization of \mathcal{I}^{AB} . Since U is a vertex cover, Lemma 7 implies that T can be extended to a realization of \mathcal{I} .
- (\Leftarrow) Let T be any realization of \mathcal{I} . By Lemma 8, T restricted to azure and beige atoms has the form (3). Lemma 3 implies that the sequence

$$\overleftarrow{\boldsymbol{\beta}}^{m0} \preceq \overleftarrow{\boldsymbol{\beta}}^{m1} \preceq \ldots \preceq \overleftarrow{\boldsymbol{\beta}}^{m(J-1)} \preceq \overleftarrow{\boldsymbol{\beta}}^{mJ},$$

(where $\boldsymbol{\beta}^{mJ} = \boldsymbol{\pi}$) has at most K(n-K) + 1 distinct vectors, and thus $\boldsymbol{\beta}^{ma} = \boldsymbol{\beta}^{m(a+1)}$ for some $0 \le a \le J - 1$. By (4), we get

$$\overleftarrow{oldsymbol{eta}}^{ma} = oldsymbol{lpha}^{ma} = \overleftarrow{oldsymbol{eta}}^{ma+1} = oldsymbol{lpha}^{ma+1} = \dots = \overleftarrow{oldsymbol{eta}}^{ma+m-1} = oldsymbol{lpha}^{ma+m-1}.$$

Define $U = \{u : \alpha_u^{am} = 0\}$. Using Lemma 7, we obtain that U is a vertex cover.

To complete the proof we note that the unary encoding of \mathcal{I} has size $O(n^{10})$, and it can be computed in polynomial time.

7 Final Comments

We proved that c-CCP is NP-complete for $c \geq 3$. Since it is known that 1-CCP can be solved efficiently in polynomial time (see [1]), the only unresolved case is for c = 2.

Relation to multicommodity flows. Consider the following problem: given a bipartite directed graph H = (U, V, E), where E is the set of arcs directed from U to V, with each arc having capacity 1, we want to ship two commodities from the vertices in U to the vertices in V, according to the given supplies in U and demands in V. More specifically, for each vertex $u_i \in U$ we are given a supply x_i^a of commodity a, and for each vertex $v_j \in V$ we are given a demand y_j^a of commodity a, where $a \in \{1, 2\}$. We wish to compute an integral 2-commodity flow from U to V of maximum total value. Let us call it 2-Commodity Integral 2-Layer Flow, or 2-CI2LF. It is known (see, [3]) that the 2-commodity integral flow problem is NP-hard for directed networks. We can improve it to the 2-layer case. By modifying the argument outlined in Section 2, it is not difficult to show that 2-CI2LF is NP-hard as well: simply note that all but two atom types have unique realizations which are independent of the given instance G, K of Vertex Cover, and associate the entries not occupied by these atoms with the edges of the resulting graph H. (Another proof can be obtained by modifying the proof in [4] in a similar fashion.)

The argument above does not imply that 2-CCP is NP-complete, since the graphs corresponding to the 2-CCP problem are *complete* bipartite graphs. This leads to the following open problem: Can 2-CI2LF be solved in polynomial time for complete bipartite graphs?

Consequences to data security problems. Similar to [4], our result has some consequences for problems arising in statistics and data security.

The reconstruction problem for contingency tables is similar to the 1-CCP problem, except that now we allow a realization to contain any non-negative integers (not just 0's and 1's). Our result implies that this problem is NP-hard even when we want to reconstruct a table whose entries are in the set $\{0, 1, \mu, \mu^2\}$, for some given μ . (To see this, modify the proof by representing each table entry in a μ -ary notation, where $\mu = L + 1$, and associate color sums with the coefficients of 1, μ and μ^2 .)

A related problem, arising in the 3D statistical data security problem, is to reconstruct a 3D table from its projections, which are called the row, column and file sums. Irving and Jerrum [7] proved that this problem is NP-hard even when all file sums are either 0 or 1. The work in [4] implies that the problem is NP-hard for $L \times L \times 7$ tables and all file sums equal 1. Our result improves this result further to tables of size $L \times L \times 4$.

References

- [1] R.A. Brualdi. Matrices of zeros and ones with fixed row and column sum vectors. *Linear Algebra and Applications*, 33:159–231, 1980.
- [2] S.-K. Chang. The reconstruction of binary patters from their projections. Communications of ACM, 14:21-24, 1971.
- [3] S. Even, A. Itai, and A. Shamir. On the complexity of timetable and multicommodity flow problems. SIAM Journal on Computing, 5(4):691–703, 1976.

- [4] R.J. Gardner, P. Gritzmann, and D. Prangenberg. On the computational complexity of determining polyatomic structures by X-rays. To appear in *Theoretical Computer Science.*, 1997.
- [5] R.J. Gardner, P. Gritzmann, and D. Prangenberg. On the computational complexity of reconstructing lattice sets from their X-rays. Technical Report 970.05012, Techn. Univ. München, Fak. f. Math., 1997.
- [6] M.R. Garey and D.S. Johnson. Computers and Intractability: A Guide to the Theory of NP-Completeness. W.H.Freeman and Co., 1979.
- [7] R.W. Irving and M.R. Jerrum. Three-dimensional statistical data security problems. SIAM Journal on Computing, 23:170–184, 1994.
- [8] C. Kisielowski, P. Schwander, F.H. Baumann, M. Seibt, Y. Kim, and A. Ourmazd. An approach to quantitate high-resolution transmission electron microscopy of crystalline materials. *Ultramicroscopy*, 58:131–155, 1995.
- [9] H.J. Ryser. Combinatorial Mathematics. Mathematical Association of America and Quinn & Boden, Rahway, New Jersey, 1963.
- [10] P. Schwander, C. Kisielowski, M. Seigt, F.H. Baumann, Y. Kim, and A. Ourmazd. Mapping projected potential, interfacial roughness, and composition in general crystalline solids by quantitative transmission electron microscopy. *Physical Review Letters*, 71:4150–4153, 1993.